A R C H I V E S O F M E T A L L U R G Y A N D M A T E R I A L S
Volume 58 2013 Issue 4
DOI: 10.2478/amm-2013-0139

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ENTALL – THERMODYNAMIC DATABASE OF ALLOYS

ENTALL – TERMODYNAMICZNA BAZA DANYCH STOPÓW

Li-Si, Ag-Ca, B-Li, Ca-Li and Al-Li belong to the group of application alloys. The Entall database includes experimental data on the enthalpy of formation of the intermetallic phases belonging to the mentioned systems, as well as software for the calculation of other thermodynamic functions. The presented Entall database is the first proposal of a thermodynamic property data, which will be gradually extended by new metal alloy systems. It is a free database, available at www.entall.imim.pl.
Keywords: Database, thermodynamic properties, hydrogen storage

Stopy Li-Si, Ag-Ca, B-Li, Ca-Li, oraz Al-Li należą do grupy stopów, mających zastosowania aplikacyjne. Baza Entall zawiera eksperymentalne dane entalpii tworzenia faz międzymetalicznych należących do cytowanych układów oraz oprogramowanie dające możliwość wyliczenia innych funkcji termodynamicznych. Prezentowana baza Entall jest pierwszą propozycją bazy właściwości termodynamicznych, która będzie stopniowo rozbudowywana o nowe układy stopów metali. Jest to baza darmowa i dostępna pod adresem www.entall.imim.pl.

1. Introduction

Since the beginning of the 1990s, in the European Union, as well as in Japan and the United States, intensified activity has been observed in the field of promoting the development of ecological technologies, such as the development of hydrogen power engineering in the context of motor industry applications as well as ecological energy sources. It should be noted that hydrogen does not exist in the unbound state and thus, in the case of its common application, it is necessary to create new technologies of its production, as well as its reprocessing to electric energy, and also, a new way of its storage. Beside the traditional methods of hydrogen storage in the form of compressed gas or liquid, it is more and more seriously considered to store it by adsorption in materials of a very strongly developed surface (e.g. Pd, Pt) and in chemical compounds, especially those in the form of hydrides. Until recently, the materials used for the hydrogen storage had almost exclusively been metals and alloys of relatively heavy elements and, as a result, their weight capacity to store hydrogen had been very low. Examples of such compounds are: TiFe, $ZrMn_2$, $LaNi_5$ and Mg_2Ni. In average, these materials can store from 1,4 to 3,6% of hydrogen [1]. A much better gravimetric capacity is possessed by the hydrides of metals of lower atomic weights, such as lithium, sodium, calcium, magnesium, silicon, aluminium as well as their alloys. Thus the world is interested in the research on their abilities to absorb and desorb hydrogen, the structure and thermodynamics, as well as the thermodynamic equilibrium modeling between metals and hydrides and between different hydrides. Taking into consideration the important energy aspects and the increasing interest in the hydrogen and energy storing metals, actions have been taken aiming at the creation of one internet application collecting the information on the thermodynamics of the discussed materials.

2. Entall database

The new database is being created on the thermodynamic properties of alloys. Currently, it includes experimental data on the enthalpy of formation of the intermetallic phases from the Li-Si [2, 3], B-Li [4] and Ca-Li [5] systems, the enthalpy of mixing for the Ca-Li system and the measurement results for the electromotive forces in the Li-Si system [6].

The Entall database has been created as a three-layer internet application, which includes the following:

1. A client internet browser,
2. An application server,
3. The database.

The database does not include figures. Each point which can appear on any diagram is represented as a separate entry (record). This allows the users to compose diagrams which precisely correspond to their expectations (e.g. to combine a few data sources on one diagram, display only that portion of the points which meets the given criterion etc.).

The Entall database includes data on the following thermodynamic properties:

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– enthalpy of solution,

– enthalpy of formation of intermetallic phases and compounds,

– enthalpy of mixing of liquid alloys,

– electromotive force measurements for solid and liquid alloys and calculated from them:

– activity of component "i",

$$a_i = e^{\frac{-n * F * E}{R * T}} \quad (1)$$

where:

n is the valence of „i" ions,

E is the emf of cell,

R is the gas constant,

T and F are the temperature and Faraday constant, respectively.

- partial molar Gibbs free energy of metal "i"

$$\Delta G_i = -n * F * E = R * T * \ln(a) \quad (2)$$

$$\Delta G_i = -n * F * E = R * T * \ln(a) = \Delta H - \Delta S * T \quad (3)$$

$$\Delta G_i = -n * F * E(T) \quad (4)$$

If the electromotive force is given in the form of a linear equation E(T)=A+BT, the other thermodynamic functions are calculated according to the following relations:

– partial enthalpy,

$$\Delta H_i = -n * F * A \quad (5)$$

– partial entropy,

$$\Delta S_i = n * F * B \quad (6)$$

– partial excess Gibbs free energy,

$$\Delta G_i^{ex} = -n * F * E - R * T * \ln(X_i) \quad (7)$$

– excess entropy,

$$S_i^{ex} = \Delta S_i + R * \ln(X_i) \quad (8)$$

– activity coefficient of metal "i",

$$\gamma_i = \frac{a_i}{X_i} \quad (9)$$

Figure 1 show the way of presenting data of enthalpy of formation in the B-Li system obtained from the calorimetric measurements.

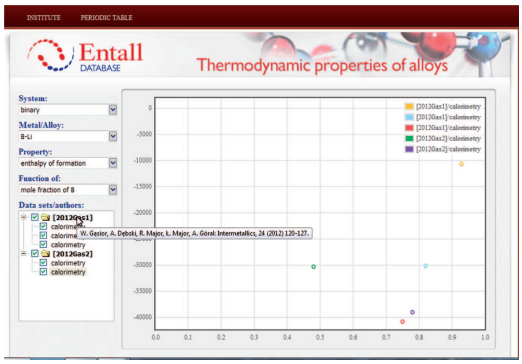

Fig. 1. Entall – enthalpy of formation of intermetallic phases from B-Li [4]

The database also makes it possible to obtain information on the method used for the determination of the given thermodynamic value as well as on the literature sources including the data applied in the creation of the diagram.

3. Conclusions

The new database of the thermodynamic properties of alloys has been created, which contains the experimental data of the enthalpy of formation of the intermetallic phases from the systems which can store hydrogen and energy, as well as the results of the electromotive force measurements.

On the basis of the electrochemical test results, it is possible to present other calculable thermodynamic functions such as: activity, activity coefficient, changes of Gibb's free energy, enthalpy and entropy, as well as excess functions.

The database is being gradually extended by new experimental thermodynamic data for other systems – not only those important for the energy storage.

An option of presenting the elaborated experimental data in the form of a Redlich-Kister equation or others is also under preparation.

It is being considered to combine the Entall thermodynamic property database with the SURDAT physicochemical property database [7], which would make it possible to obtain information on a larger number of properties and systems coming from one base.

Acknowledgements

The authors wish to express their gratitude to the Ministry of Science and Higher Education of Poland for funding Project No. IP2011 009871 "Thermodynamics of alloys for safe hydrogen storage and energy", financed from the budget for science in the years 2012-2014.

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Received: 10 April 2012.